# Replica bounds for optimization problems and diluted spin systems

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In this paper we generalize to the case of diluted spin models and random combinatorial optimization problems a technique recently introduced by Guerra (cond-mat/0205123) to prove that the replica method generates variational bounds for disordered systems. We analyze a family of models that includes the Viana-Bray model, the diluted p-spin model or random XOR-SAT problem, and the random K-SAT problem, showing that the replica method provides an improvable scheme to obtain lower bounds of the free-energy at all temperatures and of the ground state energy. In the case of K-SAT the replica method thus gives upper bounds of the satisfiability threshold.

## I. INTRODUCTION

The replica method [1,2], originally devised as a trick to compute thermodynamical quantities of physical systems in presence of quenched disorder, has found applications in the analysis of systems of very different nature, as Neural Networks, Combinatorial optimization problems [2–4], Error Correction Codes [4] etc.

Although many physicists believe that the method, within the Replica Symmetry Breaking scheme of Parisi [2], is able to potentially give the exact solution of any problem treatable as a mean field theory, the necessary mathematical foundation of the theory is still lacking, after more then 20 years from its introduction in theoretical physics. The last times have seen a growing interest of the mathematical community in the method, leading to important but still partial results, confirming in certain cases the replica analysis, with more conventional and well established techniques [5]. Apart the remarkable exception of the analysis of the fully connected p-spin model in ref. [6] and the rigorous analysis of Random Energy Models [7], the analysis of the mathematicians has been, as far as we know, restricted to the high temperature regions and/or to problem of replica symmetric nature.

Very welcomed have been the techniques recently introduced by Guerra and Toninelli [8] which allow rigorous analysis not relying on the assumption of high temperature, and valid even in problems with replica symmetry breaking. Along these lines, an important step towards the rigorous comprehension of the replica method, has been undertaken in [9], where it has been shown how in the case of the Sherrington-Kirkpatrick model, and its pspin generalizations, the replica free-energies with arbitrary number of replica symmetry breaking steps constitute variational lower bounds to the true free-energy of the model. As stated in that paper, the analysis is restricted to fully-connected models, whose replica mean field theory can be formulated in terms of a single  $n \times n$  matrix. However, in recent times, many of the more interesting problems analyzed with replica theory pertain to the so called "diluted models" where each degree of freedom interacts with a finite number of neighbors. The introduction of a "population dynamics algorithm" [10] has allowed to treat in full generality -within statistical precision- complicated sets of probabilistic functional equations appearing in the one step symmetry broken framework of diluted models. The same algorithm has been used as a starting point of a generalized "belief propagation" algorithm for optimization problems [11,12]. Furthermore, at the analytic level, simplifications due to graph homogeneities in some cases [13], and to the vanishing temperature limit in some other cases [14] have led to supposedly exact solutions of the ground state properties of diluted models, culminated in the resolution of the random XOR-SAT on uniform graphs in [13] and the random K-SAT problem in [12] within the framework of "one-step replica symmetry breaking" (1RSB).

The aim of this paper, is to show that the replica analysis of diluted models provides lower bounds for the exact free-energy density, and ground state energy density. We analyze in detail the cases of the diluted *p*-spin model on the Poissonian degree hyper-graphs also known as random XOR-SAT problem and the random K-SAT problems. We expect that along similar lines free-energy lower bounds can be found for many other diluted cases.

The Guerra method we use sheds some light on the meaning of the replica mean field theory. The physical idea behind the method is that within mean field theory one can modify the original Hamiltonian weakening the strength of the interaction couplings or removing them partially or totally, and compensate this removal by some auxiliary external fields. In disordered systems these fields should be random fields, taken from appropriate probability distributions and possibly correlated with the original values of the quenched variables eliminated from the systems. One is then led to consider Hamiltonians interpolating between the original model and a pure paramagnet in a random field, and by means of these models achieving free-energy lower bounds. We will see that the RS case corresponds to

assuming independence between the random fields and the quenched disorder. The Parisi RSB scheme, assumes at each breaking level a peculiar kind of correlations, and gives free-energy bounds improving the RS one.

Our paper is organized in this way: in section 2 we introduce some notations that will be extensively used in the following sections. In section 3 we introduce the general strategy to get the replica bounds; we then specialize to the replica symmetric and the one step replica symmetry broken bounds, giving the results in the p-spin and the K-SAT cases. Conclusions are drawn in section 4. In the appendices some details of the calculations in both the p-spin and the K-SAT cases are shown.

Our results will be issue of explicit calculations. Although at the end we will get bounds, formalizable as mathematical theorems, the style and most of the notations of the paper will be the ones of theoretical physics.

#### II. NOTATIONS

The spin models we will consider in this work are defined by a collection of N Ising  $\pm 1$  spins  $\mathbf{S} = \{S_1, ..., S_N\}$ , interacting through Hamiltonians of the kind

$$\mathcal{H}^{(\alpha)}(\mathbf{S}, \mathbf{J}) = \sum_{\mu=1}^{M} H_{J^{(\mu)}}(S_{i_1^{\mu}}, ..., S_{i_p^{\mu}})$$
(1)

where the indices  $i_l^{\mu}$  are i.i.d. quenched random variables chosen uniformly in  $\{1,...,N\}$ . We will call each term  $H_{J^{(\mu)}}$  a clause. The subscript  $J^{(\mu)}$  in the clauses indicates the dependence on a single or a set of quenched random variables, as it will be soon clear. The number of clauses M will be taken to be proportional to N. For convenience we will choose it to be for each sample a Poissonian number with distribution  $\pi(M, \alpha N) = e^{-\alpha N} \frac{(\alpha N)^M}{M!}$ . The fluctuations of M will not affect the free-energy in the thermodynamic limit, and this choice, which slightly simplify the analysis, will be equivalent to choosing a fixed value of M equal to  $\alpha N$ . The clauses themselves will be random. The p-spin model [15] has clauses of the form

$$H_{J^{(\mu)}}(S_{i_1^{\mu}}, ..., S_{i_p^{\mu}}) = J^{\mu} S_{i_1^{\mu}} \cdot ... \cdot S_{i_p^{\mu}}.$$
(2)

This form reduces to  $H_{J^{(\mu)}}(S_{i_1^{\mu}}, S_{i_2^{\mu}}) = J^{\mu}S_{i_1^{\mu}}S_{i_2^{\mu}}$  in the case of the Viana-Bray spin glass p=2. In both cases the  $J^{\mu}$  will be taken as i.i.d. random variable with regular symmetric distribution  $\mu(J) = \mu(-J)$ . Notice that for  $\mu(J) = 1/2[\delta(J+1) + \delta(J-1)]$  the model reduces to the random XOR-SAT problem [16] of computer science. The random K-SAT clauses have the form [14]

$$H_{J^{(\mu)}}(S_{i_1^{\mu}}, ..., S_{i_p^{\mu}}) = \prod_{l=1}^p \frac{1 + J_{i_l^{\mu}}^{\mu} S_{i_l^{\mu}}}{2} , \qquad (3)$$

where the  $J_{i_l}^{\mu}=\pm 1$  are i.i.d. with symmetric probability. (The number p of spin appearing in a clause is usually called K in the K-SAT problem, for uniformity of notation we will deviate from this convention). Notice that in all cases, on average each spin participate to  $\alpha=\frac{M}{N}$  clauses, and that the set of spins and interactions defines a random diluted hyper-graph of uniform rank p and random local degree with Poissonian statistics in the thermodynamic limit. At high enough temperature, the existence of the free-energy in the thermodynamic limit for models of this kind has been proved in by Talagrand in [17], together with the validity of the RS solution. A proof valid at all temperature based on the ideas presented in this paper, can be obtained for even p in analogy of the analysis in [8] for long range models. We sketch it in appendix C in the case of the p-spin model.

In establishing the free-energy bounds we will need several kind of averages:

• The Boltzmann-Gibbs average for fixed quenched disorder: given an observable  $A(\mathbf{S})$ 

$$\omega(A) = \frac{\sum_{\mathbf{S}} A(\mathbf{S}) \exp(-\beta \mathcal{H}(\mathbf{S}, \mathbf{J}))}{Z}$$
(4)

where  $Z = \sum_{\mathbf{S}} \exp(-\beta \mathcal{H}(\mathbf{S}, \mathbf{J}))$  and  $\beta$  is the inverse temperature.

Obviously,  $\omega(A)$ , as well as Z will be functions of the quenched variables, the size of the system and the temperature. This dependence will be made explicit only when needed.

- The disorder average: given an observable quantity B dependent on the quenched variables appearing in the Hamiltonian, we will denote as E(B) its average. This will include the average with respect to the J variables and the choice of the random indices in the clauses as well as with respect to other quenched variables to be introduced later.
- We will need in several occasion the "replica measure"

$$\Omega(A_1, ..., A_n) = E(\omega(A_1)...\omega(A_n))$$
(5)

and some generalizations that we will specify later.

- We will occasionally use other kinds of averages, as well as other notations, for which we will use an angular bracket notation, with a subscript indicating the variable(s) over which the average is performed. e.g. an average over a random variable u with probability distribution Q(u) will be denoted equivalently as  $\int du Q(u)(\cdot) \equiv \int dQ(u)(\cdot) \equiv \langle \cdot \rangle_u$ . Analogously, averages over distribution families of Q(u) will be denoted as  $\int dQ Q(Q)(\cdot) \equiv \int \mathcal{D}Q(Q)(\cdot) \equiv \langle \cdot \rangle_Q$ . Subscripts will be omitted whenever confusion is not possible.
- Another notation we will have the occasion to use in the one for the overlaps among l spin configurations  $\{S_i^{a_1},...,S_i^{a_l}\}$ , out of a population of n  $\{S_i^1,...,S_i^n\}$ :

$$q^{(a_1,\dots,a_l)} = \frac{1}{N} \sum_{i=1}^{N} S_i^{a_1} \cdot \dots \cdot S_i^{a_l} \quad (1 \le a_r \le n \quad \forall r), \tag{6}$$

and in particular

$$q^{(n)} = q^{(1,\dots,n)} = \frac{1}{N} \sum_{i=1}^{N} S_i^1 \cdot \dots \cdot S_i^n , \qquad (7)$$

This notation will be extended to multi-overlaps in the 1RSB case, as we will specify in section IIIB.

In the following we will need to consider averages where some of the variables are excluded, e.g. the averages when a variable  $u_i^{k_i}$  is erased. These average will be denoted with a subscript  $-u_i^{k_i}$  e.g. if an  $\omega$  average is concerned the notation will be  $\omega(\cdot)_{-u_i^{k_i}}$ . Other notations will be defined later in the text whenever needed.

Our interest will be confined to bounds to the free-energy density  $F_N = -\frac{1}{\beta N}E \log Z$  and the ground state energy density  $U_{GS} = \lim_{N\to\infty} 1/NE \left[\min\left(U_N\right)\right]$  valid in the thermodynamic limit, so that O(1/N) will be often implicitly neglected in our calculations.

## III. THE GENERAL STRATEGY

The strategy to get the replica bound is a generalization of the one introduced by Guerra in the case of fully connected models [9]. We will consider models which will interpolate between the original ones we want to analyze and pure paramagnet in random fields with suitably chosen distribution. The underlying idea is that, given the mean field nature of the models involved, if one was able to reconstruct the real local fields acting on a given spin variable via a given hyper-edge, and to introduce auxiliary fields acting on that variable in such a way to energetically balance the deletion of the hyper-edge, then it would be possible to have an exact expression for the free-energy in terms of such auxiliary fields even when the whole edge set was emptied. However, if the replacement is done with some approximate form of the auxiliary fields distribution function, the real free-energy will be the one calculated using the approximate fields plus an excess term at every step of the graph deletion process. The proof of the definite sign of this excess term gives a way to determine bounds for the thermodynamic quantities.

We will prove the existence of replica lower bounds to the free-energy density of the p-spin model and the random K-SAT problem. In this last case our result proves that the recent replica solution of [12] gives a lower bound to the ground state energy and therefore an upper bound for the satisfiability threshold. The proofs will strictly hold in the  $N \to \infty$  limit, due to the presence of corrections of order 1/N in the calculated expressions for any finite size graph. Moreover, our proofs will be restricted to the p-spin model the K-SAT with even p. In the cases of odd p the same bound would hold if one could rely on some physically reasonable assumptions on the overlap distribution (see below).

Our analysis will start from the TAP equations for the models [18,10], and their probabilistic solutions implied by the cavity, or equivalently the replica method at various degrees of approximation. We will consider in particular the replica symmetric (RS) and one step replica symmetry broken solutions, but it should be clear from our analysis how to generalize to more steps of replica symmetry breaking. In the TAP/cavity equations one singles out the contribution of the clauses and the sites to the free-energy and defines cavity fields  $h_i^{(\mu)}$  and  $u_\mu^{(i)}$  respectively as the local field acting on the spin i in absence of the clause  $\mu$  and the local field acting on i due to the presence of the clause  $\mu$  only. If we define  $Z_N[S_i]$  as the partition function of a given sample with N spins where all but the spin i are integrated,  $F_{N,-i}$  the free-energy of the corresponding systems where the spin  $S_i$  and all the clauses to which it belongs are removed, we can write,

$$Z_{N}[S_{i}] = e^{-\beta F_{N,-i}} \prod_{\mu \in T_{i}} \sum_{S_{i_{2}}^{\mu}, \dots, S_{i_{p}}^{\mu}} e^{-\beta H_{J(\mu)}(S_{i_{1}}, S_{i_{2}}^{\mu}, \dots, S_{i_{p}}^{\mu}) + \sum_{l=2}^{p} h_{i_{l}}^{(\mu)} S_{i_{l}}^{\mu}}$$

$$= e^{-\beta F_{N,-i}} \prod_{\mu \in T_{i}} B_{\mu}^{(i)} e^{\beta u_{\mu}^{(i)} S_{i}}$$
(8)

where  $T_i$  is the set of clauses containing the spin i, and the constant  $B_{\mu}^{(i)} = e^{-\beta \Delta F_{\mu}^{(i)}}$  can be interpreted as suitable shifts in the free-energy due to the contribution of the clause  $\mu$  for fixed value of the spin i. We notice that denoting  $J^{\mu}$  as J, and renaming the fields in (8) into  $h_1, ..., h_{p-1}$ , Eq. (8) defines functions

$$u_J(h_1, ..., h_{p-1})$$
 and  $B_J(h_1, ..., h_{p-1})$ . (9)

The equation are closed by the self-consistent condition:

$$h_i^{(\mu)} = \sum_{\nu \in \{T_i - \mu\}} u_\nu^{(i)} \tag{10}$$

These equations are at the basis of iterative algorithms such as the "belief propagation" or "sum-product" know for a long time in statistical inference [19] and coding theory [20] and the more recently proposed algorithm of "survey propagation" [12]. Conditions (8) and (10) can be diagrammatically represented as in fig.(1).

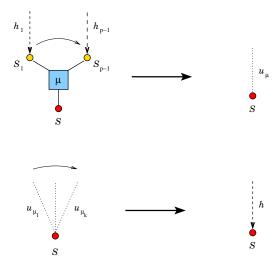


FIG. 1. Diagrammatic representation of the cavity relations for h and u fields acting on spin S. The hyper-edge interaction is drawn in the factor-graph notation.

The cavity fields solutions of (8,10) are random variables which fluctuate for two reasons [2,10,21]. First, they differ from sample to sample. Second, within the same sample the equations can have several solutions which can level-cross. The cavity/replica method provides under certain assumption probabilistic solutions. In the RS approximation, one just supposes a single solution to give the relevant contribution in a given sample. The sample to sample fluctuation induce probability distributions P(h) and Q(u) whose relations implied by (8,10) are:

$$P(h) = \sum_{k} e^{-\alpha p} \frac{(\alpha p)^{k}}{k!} \int du_{1} \ Q(u_{1}) ... du_{k} \ Q(u_{k}) \delta(h - \sum_{i=1}^{k} u_{k})$$
(11)

$$Q(u) = \int dh_1 \ P(h_1)...dh_{p-1} \ P(h_{p-1}) \langle \delta(u - u_J(h_1, ..., h_{p-1})) \rangle_J$$
 (12)

where  $\langle \cdot \rangle_J$  denotes the average over the random variables appearing in a clause. In addition to sample to sample fluctuations, the 1RSB solution assumes fluctuations of the fields from solution to solution of the equations, so that the functions P(h) and Q(u) will be themselves randomly distributed according to some functional probability distributions  $\mathcal{P}(P)$  and Q(Q) related by the self-consistency equations [22]

$$Q(Q) = \int \mathcal{D}P_1 \mathcal{P}(P_1) ... \mathcal{D}P_{p-1} \mathcal{P}(P_{p-1}) \langle \delta(Q(\cdot) - Q(\cdot | P_1, ..., P_{p-1}, J)) \rangle_J$$
(13)

$$\mathcal{P}(P) = \sum_{k=0}^{\infty} e^{-\alpha p} \frac{(\alpha p)^k}{k!} \int \prod_{l=1}^k \mathcal{D}Q_l \mathcal{Q}(Q_l) \delta(P(\cdot) - P(\cdot|Q_1, ..., Q_k))$$
(14)

where:

$$Q(u|P_1,...,P_{p-1},H) = \mathcal{N}_P[P_1,...,P_{p-1}] \int dh_1 \ P_1(h_1)...dh_{p-1} \ P_1(h_{p-1})B_{\mathbf{J}}(h_1,...,h_{p-1})^m \delta(u - u_{\mathbf{J}}(h_1,...,h_{p-1}))$$
(15)

$$P(h|Q_1, ..., Q_k) = \mathcal{N}_{Q,k}[Q_1, ..., Q_k] \left(2\cosh(\beta h)\right)^m \int \prod_{l=1}^k du_l \, \frac{Q_l(u_l)}{(2\cosh(\beta u_l))^m} \delta(h - \sum_{l=1}^k u_l)$$
(16)

where  $\mathcal{N}_{Q,k}[Q_1,...,Q_k]$  and  $\mathcal{N}_G[G_1,...,G_{p-1}]$  insure normalization and  $B_{\mathbf{J}}(g_1,...,g_{p-1})$  is a rescaling term of the form (9) that can be reabsorbed in the normalization in the case of the *p*-spin model. Its form for the *K*-SAT case is given in the appendix. m is a number in the interval (0,1], which within the formalism selects families of solutions at different free-energy levels. The physical free-energy is estimated maximizing over m.

The interpretation of these equations has been discussed many times in the literature [2,10,21]. We will show here, that such choices in the field distributions result in lower bounds for the free-energy analogous to the ones first proved by Guerra in fully connected models. In order to prove these bounds, we will have to consider auxiliary models where the number of clauses  $\alpha N$  will be reduced to  $\alpha t N$  ( $0 \le t \le 1$ ), while this reduction will be compensated in average by some external field terms of the kind:

$$\mathcal{H}_{ext}^{(t)} = \sum_{i} \sum_{l_i=1}^{k_i} u_i^{l_i} S_i \tag{17}$$

where the numbers  $k_i$  will be i.i.d. Poissonian variables with average  $\alpha p(1-t)$ . As the notation suggests, the fields  $u_i^{(i)}$  will play the role of the cavity fields  $u_\mu^{(i)}$  of the TAP approach, and they will be i.i.d. random variables with suitable distribution. Indeed, for each field  $u_i^{l_i}$  we will chose in an independent way p-1 primary fields  $g_i^{l_i,n}$  (n=1,...,p-1) and clause variables  $J_i^{l_i,n}$  such that the relation

$$u_i^{l_i} = u_{J_i^{l_i,n}}(g_i^{l_i,1}...g_i^{l_i,p-1})$$
(18)

is verified. Notice that the compound Hamiltonian

$$\mathcal{H}_{tot}^{(t)}[\mathbf{S}] = \mathcal{H}^{(\alpha t)}[\mathbf{S}] + \mathcal{H}_{ext}^{(t)}[\mathbf{S}]$$
(19)

will constitute a sample with the original distribution for t = 1, while it will consist in a system of non interacting spins for t = 0. The key step of the procedure, consists in the choice of the distribution of the primary fields  $g_i^{l_i}$ . We will also find useful to define fields  $h_i$  verifying

$$h_i = \sum_{l=1}^{k_i} u_i^l. (20)$$

The field u are related to the g's by a relation similar to (8), while the h's are related to the u's by a relation similar to (10). Of course, the statistics of the fields h and the g's do coincide in the TAP approach. It is interesting to note that the bounds we will get, are optimized precisely when their statistical ensemble coincide. As we mentioned, various Replica bounds are obtained assuming for the fields  $g_i^{l_i}$  the type of statistics implied by the different replica solution. So, the Replica Symmetric bound is got just supposing the field as quenched variables completely independent of the quenched disorder and with distribution G(g). For the one-step RSB bound on the other hand the distribution G(g) will itself be considered as random, subject to a functional probability distribution G(g). More complicated RSB estimates, not considered in this paper, can be obtained along the same lines. The case of the fully connected models considered by Guerra can be formalized in this way where the various field distributions involved are Gaussian.

## A. The RS bound

We consider in this case i.i.d. fields u and h distributed according probabilities Q(u) and P(h) verifying the following relation with the distribution Q(g) of the primary fields.

$$Q(u) = \int dg_1 \ G(g_1)...dg_{p-1} \ G(g_{p-1}) \langle \delta(u - u_J(g_1, ..., g_{p-1})) \rangle_J$$
 (21)

$$P(h) = P(h|k)\pi(k,\alpha p(1-t))$$
(22)

$$P(h|k) = \int du_1 \ Q(u_1)...du_k \ Q(u_k)\delta(h - \sum_{i=1}^k u_i)$$
(23)

The distribution G(g) will be chosen to be symmetric under change of sign of g, and regular enough for all the expression below to make sense. The RS bound can now be obtained following a procedure to the one of Guerra for the SK model, and considering the t dependent free-energy; with obvious notation:

$$F(t) = \lim_{N \to \infty} F_N(t) = \lim_{N \to \infty} -\frac{1}{\beta N} E \log Z_N(t)$$
(24)

where E represents the average over all the quenched variables, the one defining the clauses and the external fields. We then consider the t derivative of  $F_N$ 

$$\frac{d}{dt}F_N(t) = -\frac{1}{N\beta}\frac{d}{dt}E(\log Z_N). \tag{25}$$

As in [9] we will then write

$$F(1) = F(0) + \int_0^1 dt \, \frac{d}{dt} F(t) \tag{26}$$

and show, by an explicit computation, that, up to O(1/N) terms that will be systematically neglected, the expression coincides with the variational RS free-energy plus a remainder. In fortunate cases this term will have negative sign and neglecting it will immediately result in a lower bound for the free-energy. This happens in the Viana-Bray model, the p-spin and the K-SAT for even p. In the cases of odd p we were not able to prove the sign definiteness of the remainder, although as we will discuss we believe this to be the case on a physical basis.

The time derivative of F take contributions from the derivative of the distribution of the number of clauses M

$$\frac{d\pi(M, \alpha t N)}{dt} = -N\alpha(\pi(M, \alpha t N) - \pi(M - 1, \alpha t N)) \tag{27}$$

and the distribution of the number of u fields on each site

$$\frac{d\pi(k_i, \alpha p(1-t))}{dt} = \alpha p(\pi(k_i, \alpha p(1-t)) - \pi(k_i - 1, \alpha p(1-t)))$$
(28)

so that:

$$\frac{d}{dt}E\log Z(t) = -N\alpha \sum_{M} (\pi(M, \alpha t N) - \pi(M - 1, \alpha t N))E'\log Z(t) 
+\alpha p \sum_{i} \sum_{k_i} (\pi(k_i, \alpha p(1 - t)) - \pi(k_i - 1, \alpha p(1 - t)))E''_i\log Z(t)$$
(29)

where we have denoted as E' the average with respect to all the quenched variables except M and with  $E''_i$  the average with respect to all the quenched variables except  $k_i$ , and simply Z(t) the partition function of the N spin system  $Z_N(t)$ .

In the first term of (29) we can single out the M-th clause, and write  $Z(t) = Z_{-M}(t)\omega(\mathrm{e}^{-\beta H_M(S_{i_1^M},\dots,S_{i_p^M})})_{-M}$ , where by  $Z_{-M}(t)$  we denote the partition function of the system in absence of the M-th clause, and  $\omega(\cdot)_{-M}$  is the canonical average in absence of the M-th clause. In the following terms we single out the  $k_i$ -th field u term,  $Z(t) = Z_{-u_i^{k_i}}(t)\omega(\mathrm{e}^{\beta u_i^{k_i}S_i})_{-u_i^{k_i}}$ , where  $Z_{-u_i^{k_i}}(t)$  is the partition function in absence of the field  $-u_i^{k_i}$  and analogously for the average  $\omega(\cdot)_{-u_i^{k_i}}$ . Finally, rearranging all terms we find

$$\frac{d}{dt}E\log Z(t) = N\alpha \sum_{M} (\pi(M-1, \alpha t N)) E' \log[\omega(e^{-\beta H_{J(M)}(S_{i_{1}^{M}}, \dots, S_{i_{p}^{M}})})_{-M})] 
-p\alpha \sum_{i} \sum_{k_{i}} \pi(k_{i} - 1, \alpha p(1-t)) E''_{i} \log[\omega(e^{\beta u_{i}^{k_{i}} S_{i}})_{-u_{i}^{k_{i}}}].$$
(30)

where we have used  $\sum_{M} \pi(M-1, \alpha t N) E' \log Z_{-M} = \sum_{k_i} \pi(k_i - 1, \alpha p(1-t)) E''_i \log Z_{-u_i^{k_i}} = E \log Z$ . We notice at this point that the statistical ensemble defined by  $\pi(M-1, \alpha t N) E'$  can be substituted with the original one E and the average of the variables appearing in the clause we have singled out. To be more precise, we remark that the average  $\omega(\cdot)$  depends on the quenched variables  $D = \{\mathbf{J}, \mathbf{u}\}$  appearing in the Hamiltonian. Writing explicitly this dependence as  $\omega(\cdot|D)$ , and denoting as  $D_{-M}$  all the quenched variables except the ones appearing in the M-th clause, our statement is that thanks to the Poissonian distribution of M and the uniform choice of the indices of each clause,

$$\sum_{M} (\pi(M-1, \alpha t N)) E' \log[\omega(e^{-\beta H_{J(M)}(S_{i_{1}^{M}}, \dots, S_{i_{p}^{M}})} | D_{-M})] = E\left(\frac{1}{N^{p}} \sum_{i_{1}, \dots, i_{p}} \langle \log[\omega(e^{-\beta H_{J}(S_{i_{1}}, \dots, S_{i_{p}})} | D)] \rangle_{J}\right).$$
(31)

where by  $\langle \cdot \rangle_J$  we denote the average with respect to the random variables appearing in the clause. This is a crucial step in our analysis, in fact, similar considerations apply to the term in the second line of (30), which can be written as

$$\sum_{k_i} \pi(k_i - 1, \alpha p(1 - t)) E_i'' \log[\omega(e^{\beta u_i^{k_i} S_i})_{-u_i^{k_i}}] = E \left\langle \log \omega \left( e^{\beta u S_i} \right) \right\rangle_u . \tag{32}$$

The same kind of averages E and  $\omega$  appear in the two terms which can be therefore directly compared as we will do in the next section. This property, linked to the Poissonian character of the graph defined by the model would not hold for other ensembles of random graphs and the analysis would be technically more involved. Substituting in (30) we find:

$$\frac{1}{N}\frac{d}{dt}E\log Z(t) = \alpha E\left[\frac{1}{N^p}\sum_{i_1,\dots,i_p}\langle\log[\omega(e^{-\beta H(S_{i_1},\dots,S_{i_p})})]\rangle_H - \frac{p}{N}\sum_i\langle\log\omega(e^{\beta uS_i})\rangle_u\right]$$
(33)

Rearranging terms and using (26) we finally find that the free-energy  $F_N$  can be written as

$$F_N = F_{var}[G] + \int_0^1 dt \ R_{RS}[G, t] + O(1/N)$$
(34)

where  $F_{var}[G]$  coincides the expression of the variational free-energy in the replica treatment under condition  $G[h] = P[h] \, \forall \, h$  at t = 0 and  $\int_0^1 dt \, R_{RS}[G, t]$  is a remainder term. Instead of writing the formulae for general clauses, in order to keep the notations within reasonable simplicity, we specialize now to the specific cases of the p-spin model and the K-SAT. Notice that in all models

$$F[0] = -\frac{1}{\beta} \langle \log(2\cosh(\beta h)) \rangle_h|_{t=0}$$
(35)

In the case of the p-spin  $H_J(S_{i_1},...,S_{i_p})=JS_{i_1}\cdot...\cdot S_{i_p}$ . Substituting in eq.(33) and rearranging terms one immediately finds:

$$F_{var}^{p-spin}[G] = \frac{1}{\beta} \left[ \alpha \left( p \left\langle \log(\cosh \beta u) \right\rangle_{u} - \left\langle \log(\cosh \beta J) \right\rangle_{J} \right) - \left\langle \log(2 \cosh \beta h) \right\rangle_{h} + \alpha (p-1) \left\langle \log \left( 1 + \tanh(\beta J) \prod_{t=1}^{p} \tanh(\beta g_{t}) \right) \right\rangle_{\{g_{t}\}, J} \right]$$
(36)

while the remainder is the t integral of

$$R_{RS}^{p-spin}[G,t] = -\frac{\alpha}{\beta} \left[ \frac{1}{N^p} \sum_{i_1,\dots,i_p} E \left\langle \log(1 + \tanh(\beta J)\omega(S_{i_1}\dots S_{i_p})) \right\rangle_J - pE \left\langle \log(1 + \tanh(\beta u)\omega(S_i)) \right\rangle_u + (p-1)E \left\langle \log(1 + \tanh(\beta J) \prod_{t=1}^p \tanh(\beta g_p)) \right\rangle_{\{g_t\},J} \right].$$
(37)

The expression for  $F_{var}^{p-spin}[G]$  coincides with the RS free energy once extremized over the variational space of probability distributions G [23]. Terms have been properly added and subtracted in order to get a remainder which equal to zero if maximization over G is taken, and the temperature is high enough for replica symmetry to be exact [17]. As we will see, the remainder turns out to be positive.  $F_{var}^{p-spin}[G]$  is therefore, for all G for which its expression makes sense, a lower bound to the free-energy. At saturation the condition

$$G[h] = P[h]|_{t=0} \ \forall \ h \tag{38}$$

should hold, which is simply the self-consistency RS equation.

By using equation

$$E \left\langle \log(1 + \tanh(\beta u)\omega(S_i)) \right\rangle_u = E \left\langle \log(1 + \tanh(\beta J) \prod_{t=1}^{p-1} \tanh(\beta g_r)\omega(S_i)) \right\rangle_{\{g_t\}, J}$$
(39)

we can establish that the remainder is positive for even p. We expand the logarithm of the three terms in (absolutely converging) series of  $\tanh(\beta J)$ , and notice that thanks to the parity of the J and the g distributions, they will just involve negative terms. We can then take the expected value of each terms and write

$$R_{RS}^{p-spin}[G,t] = \frac{1}{\beta} \sum_{n=0}^{\infty} \langle \tanh^{2n} \beta J \rangle_J \frac{1}{n} \Omega \left[ (q^{(2n)})^p - pq^{(2n)} \langle \tanh^{2n} \beta g \rangle_g^{p-1} + (p-1) \langle \tanh^{2n} \beta g \rangle_g^p \right]$$
(40)

where we have introduced the overlap  $q^{(l)}$  and the replica measure  $\Omega$  defined in section 2. The series in (40) is an average of positive terms in the case of the Viana-Bray model p=2, where we get perfect squares, and more in general for all even p, as we can easily, starting from the observation that in this case  $x^p - pxy^{p-1} + (p-1)y^p$  is positive or zero for all  $x = q^{(2n)}$ ,  $y = \langle \tanh^{2n} \beta J \rangle_J$  real.

In the case of p odd, the same term is positive only if x is itself positive or zero. The bound of the free-energy would therefore be established if we were able to prove that the probability distributions of the  $q^{(2n)}$  has support on the positives.<sup>1</sup> This property, which tells that anti-correlated states are not possible, is physically very sound whenever the Hamiltonian is not symmetric under change of sign of all spins. In fact, one expects the probability of negative values of the overlaps to be exponentially small in the size of the system for large N. Unfortunately however we have not been able to prove this property in full generality. Notice that upon maximization on G, the results of [17] imply that the remainder is exactly equal to zero if the temperature is high enough for replica symmetry to hold.

<sup>&</sup>lt;sup>1</sup>A different sufficient condition for the series to have positive terms is that  $|\Omega(q^{(2n)})| \ge \langle \tanh(\beta g)^{2n} \rangle_g$ , but it is not clear its physical meaning.

In the case of the K-SAT, using def.(3) for the clause H, we find relation:

$$u_{\mathbf{J}}(h_1, ..., h_{p-1}) \equiv u_J(\{J_t\}, \{h_t\}) = \frac{J}{\beta} \tanh^{-1} \left[ \frac{\frac{\xi}{2} \prod_{t=1}^{p-1} \left( \frac{1+J_t \tanh(\beta h_t)}{2} \right)}{1 + \frac{\xi}{2} \prod_{t=1}^{p-1} \left( \frac{1+J_t \tanh(\beta h_t)}{2} \right)} \right], \tag{41}$$

where  $\xi \equiv e^{-\beta} - 1 < 0$ . Via direct inspection, the variational free-energy coincides with the RS expression [14]

$$F_{var}^{K-SAT}[G] = \frac{1}{\beta} \left[ \alpha(p-1) \left\langle \log \left( 1 + (e^{-\beta} - 1) \prod_{t=1}^{p} \left( \frac{1 + \tanh(\beta g_t)}{2} \right) \right) \right\rangle_{\{g_t\}, \{J_t\}} - \left\langle \log(2 \cosh(\beta h)) \right\rangle_h + \alpha p \left\langle \log(2 \cosh(\beta u)) \right\rangle_u - \alpha p \left\langle \log \left( 1 + \frac{(e^{-\beta} - 1)}{2} \prod_{t=1}^{p-1} \left( \frac{1 + \tanh(\beta g_t)}{2} \right) \right) \right\rangle_{\{g_t\}, \{J_t\}} \right]$$
(42)

while the remainder is the t integral of

$$R_{RS}^{K-SAT}[G,t] = -\frac{\alpha}{\beta} E \left[ \frac{1}{N^p} \sum_{i_1,\dots,i_p} \left\langle \log \left( 1 + (e^{-\beta} - 1)\omega (\prod_{t=1}^p \frac{1 + J_t S_{i_t}}{2}) \right) \right\rangle_{\{J_t\}} - \frac{p}{N} \sum_{i} \left\langle \log \left( 1 + \xi \omega \left( \frac{1 + J S_i}{2} \prod_{t=1}^{p-1} \frac{1 + J_t \tanh(\beta g_t)}{2} \right) \right) \right\rangle_{\{g_t\},J,\{J_t\}} + (p-1) \left\langle \log \left( 1 + \xi \prod_{t=1}^p \frac{1 + J_t \tanh(\beta g_t)}{2} \right) \right\rangle_{\{g_t\},\{J_t\}} \right].$$
(43)

Considerations analogous to the case of the p-spin, have led us to add and subtract terms from eq.(33) to single out the proper remainder term. Expanding in series the logarithms, exploiting the symmetry of the probabilities distribution functions and taking the expectation of each term of the absolutely convergent series we finally obtain:

$$R_{RS}^{K-SAT}[G,t] = \frac{\alpha}{\beta} \sum_{n \ge 1} \frac{(-1)^n}{n} (\xi^*)^n \Omega \left[ (1+Q_n)^p - p(1+Q_n) \langle (1+J\tanh(\beta g))^n \rangle_{J,g}^{p-1} + (p-1) \langle (1+J\tanh(\beta g))^n \rangle_{J,g}^p \right]$$
(44)

where we have defined  $\xi^* \equiv \xi/(2^p) < 0$  and  $Q_n \equiv \sum_{l=1}^n \langle J^l \rangle_J \sum_{a_1 < \dots < a_l}^{1,n} q^{a_1 \dots a_l}$ . Detailed calculations are given in the appendix. As in the *p*-spin case, the previous sum is obviously positive for *p* even. For *p* odd we should again rely on the physical wisdom that all  $q^{(a_1,\dots,a_l)}$  have positive support and so have the functions  $1+Q_n \geq 0$ . Again, the variational free-energy coincides with the RS expression once extremized over *G* at the condition P = G at t = 0.

## B. The 1RSB Bound

We establish here a more complex estimate, in a larger variational space of functional probability distributions. The general strategy will be here to consider the same form for the auxiliary Hamiltonian, but now with a more involved choice for the fields distribution. The fields on different sites or different index  $l_i$  will be still independent, but each site field distribution  $G_i^{l_i}(g_i^{l_i})$  will be itself random i.i.d., chosen with a probability density functional  $\mathcal{G}[G]$ , with support on symmetric distributions G(-g) = G(g). It will be assumed that  $\mathcal{G}$  is such that all the expressions below make sense. In this case, the variational approximation for the free-energy will be obtained from an estimate of

$$-\beta F_N[m,t] = \frac{1}{mN} E_1 \log E_2(Z^m(t))$$
(45)

where we have denoted with:

•  $E_2$  the average w.r.t.  $g_i^{l_i,n}$  for fixed distributions  $G_i^{l_i,n}$  according to the measure

$$C \prod_{i=1}^{N} \prod_{l_{i}=1}^{k_{i}} \prod_{n=1}^{p-1} dg_{i}^{l_{i},n} G_{i}^{l_{i},n}(g_{i}^{l_{i},n}) \left( \frac{B_{J_{i}^{l_{i},n}}(g_{i}^{l_{i},1}...g_{i}^{l_{i},1}...g_{i}^{l_{i},p-1})}{2 \cosh(\beta u_{J_{i}^{l_{i},n}}(g_{i}^{l_{i},1}...g_{i}^{l_{i},p-1}))} \right)^{m}$$

$$(46)$$

where C ensures the normalization.

•  $E_1$  the average with respect to the quenched clause variable, distributions the  $G_i^{l_i}$ 's and the Poissonian variables  $k_i$ 's, which will be i.i.d. with probabilities  $\mu(J)$ ,  $\mathcal{G}(G_i^{l_i})$  and  $\pi(k_i, (1-t)\alpha)$  respectively.

The number m is real in the interval (0,1]. The statistical ensemble of the auxiliary fields u and h will be now related to the one of the g by:

$$Q(Q) = \int \mathcal{D}G_1 \mathcal{G}(G_1) ... \mathcal{D}G_{p-1} \mathcal{G}(G_{p-1}) \langle \delta(Q(\cdot) - Q(\cdot | G_1, ..., G_{p-1}, J)) \rangle_J$$

$$(47)$$

$$\mathcal{P}(P) = \sum_{k=0}^{\infty} e^{-\alpha p(1-t)} \frac{(\alpha p(1-t))^k}{k!} \int \prod_{l=1}^k \mathcal{D}Q_l \mathcal{Q}(Q_l) \delta(P(\cdot) - P(\cdot|Q_1, ..., Q_k))$$

$$\tag{48}$$

where:

$$Q(u|G_1,...,G_{p-1},J) = \mathcal{N}_G[G_1,...,G_{p-1}] \int dg_1 \ G_1(g_1)...dg_{p-1} \ G_1(g_{p-1})B_J(g_1,...,g_{p-1})^m \delta(u - u_J(g_1,...,g_{p-1}))$$
(49)

$$G(g|Q_1, ..., Q_k) = \mathcal{N}_{Q,k}[Q_1, ..., Q_k] \left(2\cosh(\beta g)\right)^m \int \prod_{l=1}^k du_l \, \frac{Q_l(u_l)}{(2\cosh(\beta u_l))^m} \delta(g - \sum_{l=1}^k u_l)$$
(50)

where  $\mathcal{N}_{Q,k}[Q_1,...,Q_k]$ ,  $\mathcal{N}_G[G_1,...,G_{p-1}]$  and  $B_J(g_1,...,g_{p-1})$  have been previously defined. With notations similar to the ones of the RS case, we can write

$$\frac{d}{dt}(-\beta F_N[m,t]) = -\alpha \sum_{M} (\pi(M,\alpha tN) - \pi(M-1,\alpha tN)) E_1' \frac{1}{Nm} \log E_2 Z(t)^m 
+ \frac{\alpha p}{N} \sum_{i} \sum_{k_i} (\pi(k_i,\alpha p(1-t)) - \pi(k_i-1,\alpha p(1-t))) E_{1,i}'' \frac{1}{Nm} \log E_2 Z(t)^m$$
(51)

which, extracting explicitly the contribution from the M-th close in the first term and the  $k_i$ -th field u in the second, following considerations similar to the RS case we find:

$$\frac{d}{dt}(-\beta F_N[m,t]) = \alpha \sum_{M} (\pi(M-1,\alpha tN)) \frac{1}{m} E_1' \log \left[ \frac{E_2 Z_{-M}^m \omega(e^{-\beta H_{J(\mu)}(S_{i_1^M},...,S_{i_p^M})})_{-M}^m}{E_2 Z_{-M}^m} \right] - \frac{p\alpha}{N} \sum_{i} \sum_{k_i} \pi(k_i - 1,\alpha p(1-t)) \frac{1}{m} E_{1,i}'' \log \left[ \frac{E_2 Z_{-u_i^{k_i}}^m \omega(e^{\beta u_i^{k_i} S_i})_{-u_i^{k_i}}^m}{E_2 Z_{-u_i^{k_i}}^m} \right].$$
(52)

Again it can be recognized that the primed averages coincide with the averages over the original ensembles plus the averages on the variables appearing in the terms we extracted. Finally we get:

$$\frac{d}{dt}(-\beta F_N[m,t]) = \frac{\alpha}{m} E_1 \left[ \frac{1}{N^p} \sum_{i_1,\dots,i_p} \left\langle \log \left( \frac{E_2 Z^m \omega (e^{-\beta H_J(S_{i_1},\dots,S_{i_p})})^m}{E_2 Z^m} \right) \right\rangle_J - \frac{p}{N} \sum_i \left\langle \log \left( \frac{E_2 Z^m \langle \omega (e^{\beta u S_i})^m \rangle_u}{E_2 Z^m} \right) \right\rangle_Q \right] .$$
(53)

Rearranging all terms one finds the estimate:

$$F_N = F_{var}[\mathcal{G}] + \int_0^1 dt \ R_{1RSB}[\mathcal{G}, t] + O(1/N)$$
 (54)

where this time  $F_{var}[\mathcal{G}]$  coincides with  $F_{1RSB}[\mathcal{G}]$ , the expression of the variational free-energy in the 1RSB treatment at the saddle point  $\mathcal{G} = \mathcal{P}$  at t = 0, and  $\int_0^1 dt \ R_{1RSB}[\mathcal{G}, t]$  is the remainder. Notice that the derivation immediately suggests how to generalize the analysis to more steps of replica symmetry breaking. Let us now specialize the formulae for the p-spin model and the K-SAT. Again, in this case we will need the expression for F[0]:

$$F[0] = \frac{1}{\beta m} \left[ \left\langle \log \left\langle \left( \frac{1}{2 \cosh(\beta h)} \right)^m \right\rangle_h \right\rangle_P \right]_{t=0} . \tag{55}$$

1. p-spin

In this case, plugging def.(2) in eq.(53) rearranging, adding and subtracting terms one finds:

$$F_{var}^{p-spin}[\mathcal{G}] = \frac{1}{\beta m} \left[ \left\langle \log \left\langle \left( \frac{1}{2 \cosh(\beta h)} \right)^m \right\rangle_h \right\rangle_P - \alpha m \left\langle \log(2 \cosh(\beta J)) \right\rangle_J - \alpha p \left\langle \log \left\langle \left( \frac{1}{2 \cosh(\beta u)} \right)^m \right\rangle_u \right\rangle_Q + \alpha (p-1) \left\langle \log \left\langle (1 + \tanh(\beta J) \tanh(\beta g_1) ... \tanh(\beta g_p))^m \right\rangle_{g_1, ..., g_p} \right\rangle_{G_1, ..., G_{p; J}} \right]$$

$$(56)$$

while the remainder is the t integral of

$$R_{1RSB}^{p-spin}[\mathcal{G},t] = -\frac{\alpha}{\beta m} E_1 \left[ \frac{1}{N^p} \sum_{i_1,\dots,i_p} \left\langle \log \left( \frac{E_2 Z^m (1 + \omega(S_{i_1} \dots S_{i_p}) \tanh(\beta J))^m}{E_2 Z^m} \right) \right\rangle_J - \frac{p}{N} \sum_i \left\langle \log \left( \frac{E_2 Z^m \left\langle (1 + \omega(S_i) \tanh(\beta u))^m \right\rangle_u}{E_2 Z^m} \right) \right\rangle_Q + (p-1) \left\langle \log \left\langle (1 + \tanh(\beta J) \tanh(\beta g_1) \dots \tanh(\beta g_p))^m \right\rangle_{g_1,\dots,g_p} \right\rangle_{G_1,\dots,G_p;J} \right]$$
(57)

The expression for  $F_{var}^{p-spin}[\mathcal{G}]$  coincides with the 1RSB free-energy [23] once maximized over the variational space of probability distribution functionals  $\mathcal{G}$ . The maximization condition reads:

$$\mathcal{G}[P] = \mathcal{P}[P] \mid_{t=0} \forall P , \qquad (58)$$

which is simply the self consistency 1RSB condition. For even p (and in particular for p=2 that corresponds to the Viana-Bray case), one can check that the remainder is positive just expanding the logarithm in series and exploiting the parity of the J and the g distributions. As this is considerably more involved then in the RS case, we relegate this check to appendix A.

2. K-SAT

In the K-SAT case the expression for function  $B_{\mathbf{J}}(h_1,...,h_{p-1})$  reads:

$$B_{\mathbf{J}}(h_1, ..., h_{p-1}) \equiv B(\{J_t\}, \{h_t\}) = 1 + \frac{\xi}{2} \prod_{t=1}^{p-1} \left( \frac{1 + J_t \tanh(\beta h_t)}{2} \right) , \tag{59}$$

while the corresponding one for  $u_{\mathbf{J}}(h_1,...,h_{p-1})$  is the same as in the RS case. The corresponding replica free-energy and remainder read

$$F_{var}^{K-SAT}[\mathcal{G}] = \frac{1}{m\beta} \left[ \alpha(p-1) \left\langle \log \left\langle \left( 1 + \xi \prod_{t=1}^{p} \left( \frac{1 + J_t \tanh(\beta g_t)}{2} \right) \right)^m \right\rangle_{\{g_t\}} \right\rangle_{\{G_t\}, \{J_t\}} - \alpha p \left\langle \log \left\langle \left( \frac{B(\{J_t\}, \{g_t\})}{2 \cosh(\beta u_J(\{J_t\}, \{g_t\}))} \right)^m \right\rangle_{\{g_t\}} \right\rangle_{\{G_t\}, \{J_t\}, J} + \left\langle \log \left\langle \left( \frac{1}{2 \cosh(\beta h)} \right)^m \right\rangle_{h} \right\rangle_{P} \right]$$
(60)

The remainder is the t integral of

$$R_{1RSB}^{K-SAT}[\mathcal{G}, t] = -\frac{\alpha}{\beta m} E_1 \left[ \frac{1}{N^p} \sum_{i_1, \dots, i_p} \left\langle \log \left( \frac{E_2 Z^m \left( 1 + \xi \omega \left( \prod_{t=1}^p \frac{1 + J_t S_{i_t}}{2} \right) \right)^m}{E_2 Z^m} \right) \right\rangle_{\{J_t\}} - \frac{p}{N} \sum_{i} \left\langle \log \left( \frac{E_2 Z^m \left\langle \left( 1 + \xi \frac{1 + J\omega(S_i)}{2} \prod_{t=1}^{p-1} \frac{1 + J_t \tanh(\beta g_t)}{2} \right)^m \right\rangle_{\{g_t\}}}{E_2 Z^m} \right) \right\rangle_{\{G_t\}, \{J_t\}, J} + (p-1) \left\langle \log \left\langle \left( 1 + \xi \prod_{t=1}^p \left( \frac{1 + J_t \tanh(\beta g_t)}{2} \right) \right)^m \right\rangle_{\{g_t\}, \{J_t\}} \right\} \right\}$$

$$(61)$$

The expression for  $F_{var}^{K-SAT}[\mathcal{G}]$  coincides with the 1RSB free energy once extremized under condition (58), with the corresponding K-SAT probability distribution functionals. Notice that The proof of the positivity of (61) for even p is again dove via series expansion, all the detail are explained in Appendix B.

At this point we can take the zero temperature limit, finding that the resulting expression gives us a lower bound for the ground-state energy of the system, i.e. the minimal number of unsatisfied clauses. Notice that the  $T \to 0$  limit of the replica free-energy is not trivial. The necessary assumptions on the field distributions to get it correct are well known in the physical literature, and have been recently reviewed in [21]. Recently Mezard, Parisi and Zecchina [12] have worked out the K-SAT 1RSB solution for p=3 predicting a non zero ground-state energy for values of  $\alpha$  above a satisfiability threshold of  $\alpha_c=4.256$ , very well in agreement with the numerical simulations. Our results, together with the additional hypothesis of positivity of the support of the overlap functions imply that this value is an upper bound to the true threshold.

#### IV. SUMMARY AND CONCLUSIONS

In this paper we have established that the free-energy of some families of diluted random spin models can be written as the sum of a term identical to the ones got in the cavity/replica plus an error term. Both the replica term and the remainder are different in different replica scheme, corresponding to the choice of statistical ensemble of the cavity fields. We believe that the sign of the remainder is in general negative in the model we have considered, although we have been able to prove that only in the case of even p. For odd p our belief is supported by the physical wisdom that the overlap distributions are supported on the positives in the large N limit.

We have considered the cases of replica symmetry and one step of replica symmetry breaking. It is clear that the analysis could be extended to further levels of replica symmetry breaking, although the complexity of the analysis would greatly increase. The 1RSB level is thought to give the exact scheme to treat the p spin model and the K-SAT problem for  $p \geq 3$ . For the Viana-Bray model on the other hand it is believed that no finite RSB scheme furnish the exact solution, and one needs to consider the limit of infinite number of replica symmetry breaking. It is not clear to us how to generalize the analysis to this case.

Our analysis of the diluted models underlines a strong link between the Guerra method and the cavity method which remained rather hidden in the fully connected case. In the cavity approach one considers incomplete graphs in which either sites or clauses are removed from the complete graph. Then, with the aid of precise physical hypothesis, consistency equations are written that allow to compute the free-energy from the comparison between the site and clause contributions. In the approach presented in this paper the removal of clauses is compensated in average by the addition of some external fields which have precisely the statistics which is assumed with cavity. The novelty of the approach is that it gives some control on the approximation involved, and proves the variational nature of the replica free-energies. Of course a complete control on the remainder in various situations would result in rigorous solutions.

Although in this paper we have mainly worked at finite temperature, the zero temperature limit can be considered without harm. This is particularly relevant in random satisfiability problem, where it is typically found a SAT-UNSAT transition where the ground state energy passes from zero to non zero values. Our analysis shows that, the replica estimates for many of the models considered in the literature, and possibly some of the ones to be obtained in the future with the same method provide upper bounds for the satisfiability thresholds.

In this paper we have confined ourselves to spin models on graphs with Poissonian connectivity. The extension to more general diluted graph models will be presented in a forthcoming paper.

Finally we would like to remark that despite the heavy formalism, our proofs to the bounds are conceptually simple. They are issue of explicit computations and elementary positivity consideration. We hope that this contributes to illustrate the elegance of the construction first introduced in [9].

### V. ACKNOWLEDGMENTS

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#### APPENDIX A: P-SPIN

## 1. Check of the positive sign of $R_{1RSR}^{p-spin}$

In this appendix we will explicitly show that expression (57) has positive sign. We proceed expanding in absolutely convergent series each of the three addend in (57) and showing, taking the expectation of each term that the resulting series is positive semidefinite.

The first term writes:

$$E_{1} \left\langle \log \frac{E_{2}Z^{m}(1+\tanh(\beta J)\omega(S_{i_{1}}...S_{i_{p}}))^{m}}{E_{2}Z^{m}} \right\rangle_{J} = \sum_{l \geq 1} \frac{(-1)^{l+1}}{l} \sum_{k_{1},...,k_{l}}^{1,\infty} \left( \frac{m(-1)^{k_{1}-1}}{k_{1}!} \prod_{r_{1}=1}^{k_{1}-1} (r_{1}-m) \right) ... \left( \frac{m(-1)^{k_{l}-1}}{k_{l}!} \prod_{r_{l}=1}^{k_{l}-1} (r_{l}-m) \right) \left\langle (\tanh(\beta J)^{\sum_{s=1}^{l} k_{s}} \right\rangle_{J}.$$

$$E_{1} \left( \prod_{s=1}^{l} \frac{E_{2}(Z^{m}\omega(S_{i_{1}}...S_{i_{p}})^{k_{s}})}{E_{2}(Z^{m})} \right)$$
(A1)

where the term  $E_1(\cdot)$  in the last line of eq.(A1) can be written as

$$E_{1}\left(\frac{E_{2}^{(1)}...E_{2}^{(l)}Z_{(1)}^{m}...Z_{(l)}^{m}\omega_{(1)}(S_{i_{1}}^{1,1}...S_{i_{p}}^{1,1}...S_{i_{1}}^{k_{1},1}...S_{i_{p}}^{k_{1},1})...\omega_{(l)}(S_{i_{1}}^{1,l}...S_{i_{p}}^{1,l}...S_{i_{p}}^{k_{l},l}...S_{i_{p}}^{k_{l},l})}{(E_{2}Z^{m})^{l}}\right) = \Omega^{(l)}\left[(q^{(k_{1},...,k_{l})})^{p}\right]. \quad (A2)$$

where each  $\omega_{(s)}$  (s = 1, ..., l) is a product of  $k_s$  Gibbs measure with independent fields (variables appearing in the  $E_2^{(s)}$  averages), and same fields distributions and quenched disorder (variables appearing in  $E_1$ ). The quantities  $q^{(k_1, ..., k_l)}$  have been defined as:

$$q^{(k_1,\dots,k_l)} = \frac{1}{N} \sum_{i} S_i^{1,1} \cdot \dots \cdot S_i^{k_1,1} \cdot \dots \cdot S_i^{1,l} \cdot \dots \cdot S_i^{k_l,l}$$
(A3)

and in this case the averages are performed using a a generalized replica measure, defined as:

$$\Omega^{(l)}[(q^{(k_1,\dots,k_l)})^n] = E_1 \left[ \frac{\prod_{s=1}^l E_2^{(s)} Z_{(s)}^m \omega_{(s)} (S_{i_1} \dots S_{i_n})^{k_s}}{(E_2 Z^m)^l} \right]$$
(A4)

for any integer n. The average over J selects the terms with even  $\sum_{s=1}^{l} k_l$  in (A1) so that we finally find

$$-\sum_{l\geq 1} \frac{m^l}{l} \sum_{\substack{k_1,\dots,k_l\\\sum_{s=1}^l k_s \text{ even}}}^{1,\infty} \prod_{s=1}^l \left( \frac{\prod_{r_s=1}^{k_s-1} (r_s-m)}{k_s!} \right) \left\langle (\tanh(\beta J))^{\sum_{s=1}^l k_s} \right\rangle_J \Omega^{(l)} \left[ (q^{(k_1,\dots,k_l)})^p \right]$$
(A5)

notice that  $(r_s - m) \ge 0 \ \forall$  integer  $r_s > 0$  only in the current hypothesis that  $m \in [0, 1]$ . Analogously, the term

$$E_1 \left\langle \log \frac{E_2 Z^m \left\langle (1 + \tanh(\beta u)\omega(S_i))^m \right\rangle_u}{E_2 Z^m} \right\rangle_Q \tag{A6}$$

writes

$$-\sum_{l\geq 1} \frac{m^l}{l} \sum_{\substack{k_1,\dots,k_l\\\sum_{s=1}^l k_s \text{ even}}}^{1,\infty} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \left\langle \prod_{s=1}^l \left\langle \tanh(\beta u)^{k_s} \right\rangle_u \right\rangle_Q \Omega^{(l)} \left[ (q^{(k_1,\dots,k_l)}) \right]$$
(A7)

or, making use of the definition of G(g),

$$-\sum_{l\geq 1} \frac{1}{l} \sum_{\substack{k_1,\dots,k_l\\ \sum_{s=1}^{l} k_s \text{ even}}}^{1,\infty} \prod_{s=1}^{l} \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \left\langle \prod_{s=1}^{l} \left\langle (\tanh(\beta g))^{k_s} \right\rangle_g \right\rangle_G^{p-1} \left\langle (\tanh(\beta J))^{\sum_{s=1}^{l} k_s} \right\rangle_J \Omega^{(l)} \left[ (q^{(k_1,\dots,k_l)}) \right]$$
(A8)

Eventually, following analogous manipulations, the last term

$$\left\langle \log \left\langle \left( 1 + \tanh(\beta J) \prod_{t=1}^{p} \tanh(\beta g_{t}) \right)^{m} \right\rangle_{\{g_{t}\}} \right\rangle_{J,\{G_{t}\}}$$
(A9)

can be written as

$$-\sum_{l\geq 1} \frac{m^l}{l} \sum_{\substack{k_1,\dots,k_l\\\sum_{s=1}^l k_s \text{ even}}}^{1,\infty} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \left\langle \prod_{s=1}^l \left\langle (\tanh(\beta g))^{k_s} \right\rangle_g \right\rangle_G^p \left\langle (\tanh(\beta J))^{\sum_{s=1}^l k_s} \right\rangle_J. \tag{A10}$$

Invoking 47 and collecting all

$$R_{1RSB}^{p-spin}[\mathcal{G},t] = \frac{\alpha}{\beta m} \sum_{l \ge 1} \frac{m^l}{l} \sum_{\substack{k_1, \dots, k_l \\ \sum_{s=1}^l k_s \text{ even}}}^{1,\infty} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \left\langle (\tanh(\beta J))^{\sum_{s=1}^l k_s} \right\rangle_J .$$

$$\Omega^{(l)} \left[ (q^{(k_1, \dots, k_l)})^p - pA(k_1, \dots, k_l)^{p-1} (q^{(k_1, \dots, k_l)}) + (p-1)A(k_1, \dots, k_l)l^p \right]$$
(A11)

where we have defined:

$$A(k_1, ..., k_l) \equiv \left\langle \prod_{s=1}^l \left\langle (\tanh(\beta g))^{k_s} \right\rangle_g \right\rangle_G \tag{A12}$$

Each inner term of the series (A11)

$$\Omega^{(l)} \left[ (q^{(k_1, \dots, k_l)})^p - pA(k_1, \dots, k_l)^{p-1} (q^{(k_1, \dots, k_l)}) + (p-1)A(k_1, \dots, k_l)^p \right]$$
(A13)

is always positive semidefinite for p even while we need the condition conditions  $q^{(k_1,\ldots,k_l)} \geq 0$  for p odd. For p=2 one retrieves the Viana-Bray result where (A13) is a perfect square. As in the RS case, one can now integrate eq.(A11) and recognize that once more the total true free-energy can be written as variational term plus a positive extra one. The variational term coincides with the 1RSB free-energy at stationarity and under condition

$$\mathcal{G}(P) = \mathcal{P}(P)|_{t=0} \quad \forall \ P \ . \tag{A14}$$

### APPENDIX B: K-SAT

1. Check of the positive sign of  $R_{RS}^{K-SAT}$  ...

The aim of this appendix is to show that the expression for the remainder  $R_{RS}[G, t]$  in (34) for the K-SAT model case as positive sign. For the K-SAT  $R_{RS}[G, t]$  specializes to:<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>The sum of the site indices has been eliminated by symmetry.

$$R_{RS}^{K-SAT}[G,t] = -\frac{\alpha}{\beta} E\left[\left\langle \log\left(\omega\left(\exp^{-\beta}\prod_{r=1}^{p}\frac{1+J_{r}S_{r}}{2}\right)\right)\right\rangle_{\{J_{t}\}} - p\left\langle \log\left(1+\omega(S)\tanh(\beta u)\right)\right\rangle_{u} - -p\left\langle \log\left(1+\frac{\xi}{2}\prod_{t=1}^{p-1}\left(\frac{1+J_{t}\tanh(\beta g_{t})}{2}\right)\right)\right\rangle_{\{g_{t}\},\{J_{t}\}} + (p-1)\left\langle \log\left(1+\xi\prod_{t=1}^{p}\frac{1+J_{r}\tanh(\beta g_{t})}{2}\right)\right\rangle_{\{g_{t}\},\{J_{t}\}}\right]$$
(B1)

which thanks to the relation between Q(u) and G(g), rewrites as

$$R_{RS}^{K-SAT}[G,t] = -\frac{\alpha}{\beta} E\left[\left\langle \log\left(1 + (e^{-\beta} - 1)\omega(\prod_{t=1}^{p} \frac{1 + J_t S_t}{2})\right)\right\rangle_{\{J_t\}} - p\left\langle \log\left(1 + \xi\omega\left(\frac{1 + JS}{2}\prod_{t=1}^{p-1} \frac{1 + J_t \tanh(\beta g_t)}{2}\right)\right)\right\rangle_{\{g_t\}, J, \{J_t\}} + (p-1)\left\langle \log\left(1 + \xi\prod_{t=1}^{p} \frac{1 + J_t \tanh(\beta g_t)}{2}\right)\right\rangle_{\{g_t\}, \{J_t\}}\right]$$
(B2)

The last term has been added and subtracted from eq.(34) in order to extract a remainder that would vanish if replica symmetry holds, and maximization is performed on G(g). As in the *p*-spin case, we will proceed in a Taylor expansion of expression (B2) in powers of  $\xi$ , and rely on absolute convergence to average each term of the series.

Expanding the first term in (B2) we can write

$$E\left[\left\langle \log\left(1+\xi\omega(\prod_{t=1}^{p}\frac{1+J_{t}S_{t}}{2})\right)\right\rangle_{\{J_{t}\}}\right] = \sum_{n\geq 1} \frac{(-1)^{n+1}}{n} (\xi^{*})^{n} E\left[\left\langle \omega\left(\prod_{t=1}^{p}(1+J_{t}S_{t})\right)^{n}\right\rangle_{\{J_{t}\}}\right] = \sum_{n\geq 1} \frac{(-1)^{n+1}}{n} (\xi^{*})^{n} \Omega\left[\prod_{t=1}^{p}\left(1+\sum_{l=1}^{n}\left\langle J_{t}^{l}\right\rangle_{J_{t}}\sum_{a_{1}<...< a_{l}}^{1,n}S_{t}^{a_{1}}...S_{t}^{a_{l}}\right)\right] = \sum_{n\geq 1} \frac{(-1)^{n+1}}{n} (\xi^{*})^{n} \Omega\left[\prod_{t=1}^{p}\left(1+\sum_{l=1}^{n}\left\langle J_{t}^{l}\right\rangle_{J_{t}}\sum_{a_{1}<...< a_{l}}^{1,n}q^{a_{1}...a_{l}}\right)\right] = \sum_{n\geq 1} \frac{(-1)^{n+1}}{n} (\xi^{*})^{n} \Omega[(1+Q_{n})^{p}]$$
(B3)

where we have defined  $\xi^* \equiv (e^{-\beta} - 1)/(2^p)$  and  $\sum_{l=1}^n \langle J^l \rangle_J \sum_{a_1 < \dots < a_l}^{1,n} q^{a_1 \dots a_l} \equiv Q_n$ . Notice that due to the negative sign of  $\xi^*$ , the coefficients  $(-1)^{n+1}(\xi^*)^n$  are all negative.

The analogous expansion of the second term is:

$$E\left[\left\langle \log\left(1+\xi\omega\left(\frac{1+JS}{2}\prod_{t=1}^{p-1}\frac{1+J_{t}\tanh(\beta g_{t})}{2}\right)\right)\right\rangle_{\{J_{t}\},J_{t}\{g_{t}\}}\right] = \sum_{n\geq 1}\frac{(-1)^{n+1}}{n}(\xi^{*})^{n}\Omega\left[\left(1+\sum_{l=1}^{n}\langle J^{l}\rangle_{J}\sum_{a_{1}<...< a_{l}}^{1,n}q^{a_{1}...a_{l}}\right)\left\langle\prod_{t=1}^{p-1}\prod_{l=1}^{n}\left(1+J_{t}\tanh(\beta g_{t})\right)\right\rangle_{\{J_{t}\},\{g_{t}\}}\right] = \sum_{n\geq 1}\frac{(-1)^{n+1}}{n}(\xi^{*})^{n}\Omega\left[\left(1+Q_{n}\right)\langle(1+J\tanh(\beta g))^{n}\rangle_{J,g}^{p-1}\right]$$
(B4)

Finally, the third terms in eq.(B2) immediately reads

$$\left\langle \log \left( 1 + \xi \prod_{t=1}^{p} \frac{1 + J_t \tanh(\beta g_t)}{2} \right) \right\rangle_{\{J_t\}, \{g_t\}} = \sum_{n \ge 1} \frac{(-1)^{n+1}}{n} (\xi^*)^n \langle (1 + J \tanh(\beta g))^n \rangle_{J,g}^p$$
 (B5)

The sum of the three pieces in eq.(B2) gives:

$$R_{RS}^{K-SAT}[G,t] = \frac{\alpha}{\beta} \sum_{n \ge 1} \frac{(-1)^n}{n} (\xi^*)^n \Omega \left[ (1+Q_n)^p - p(1+Q_n) \langle (1+J\tanh(\beta g))^n \rangle_{J,g}^{p-1} + (p-1) \langle (1+J\tanh(\beta g))^n \rangle_{J,g}^p \right]$$
(B6)

The previous sum is always positive semidefinite for p even while we need  $1 + Q_n \ge 0$  for p odd.

2. ...and of 
$$R_{1RSB}^{K-SAT}$$

We proceed in the same way as in the p-spin case. The algebra is elementary but more tedious and involved, therefore we will only list the final results of the calculation. Starting from eq.(61), we again expand in series the first term, getting, with a treatment similar to the RS case:

$$R_{1RSB}^{K-SAT}[\mathcal{G}, t] = \sum_{l>1} \frac{m^l}{l} \sum_{k_1, \dots, k_l}^{1, \infty} (-\xi^*)^{\sum_{s=1}^l k_s} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \Omega^{(l)} \left[ (1 + \mathbf{Q}(k_1, \dots, k_l))^p \right]$$
(B7)

where we have defined:

$$\mathbf{Q}(k_1, ..., k_l) \equiv \sum_{s=1}^{l} \sum_{r_1, ..., r_s}^{k_1, ..., k_s} \left\langle J^{(r_1 + ... + r_s)} \right\rangle_J \prod_{t=1}^{s} \sum_{a_1 < ... < a_{r_t} = 1}^{k_1, ..., k_s} q^{(a_{r_1}, ..., a_{r_s})}$$
(B8)

Analogous steps give for the second term in eq.(61)

$$\sum_{l\geq 1} \frac{m^l}{l} \sum_{k_1,...,k_l}^{1,\infty} (-\xi^*)^{\sum_{s=1}^l k_s} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \Omega^{(l)} \left[ 1 + \mathbf{Q}(k_1,...,k_l) \right] \left\langle \prod_{s=1}^l \left\langle (1 + J \tanh(\beta g))^{k_l} \right\rangle_g \right\rangle_{G,J}^{p-1}$$
(B9)

and for the third term

$$\sum_{l\geq 1} \frac{m^l}{l} \sum_{k_1,\dots,k_l}^{1,\infty} (-\xi^*)^{\sum_{s=1}^l k_s} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \left\langle \prod_{s=1}^l \left\langle (1+J\tanh(\beta g))^{k_l} \right\rangle_g \right\rangle_{G,J}^p , \tag{B10}$$

where in the last two terms we can further expand

$$\left\langle \prod_{s=1}^{l} \left\langle (1 + J \tanh(\beta g))^{k_l} \right\rangle_g \right\rangle_{G,J}^n = \left( \sum_{r_1,\dots,r_l=1}^{k_1,\dots,k_l} \prod_{s=1}^{l} \binom{k_s}{r_s} \left\langle J^{(r_1+\dots+r_l)} \right\rangle_J \left\langle \prod_{s=1}^{l} \left\langle (\tanh(\beta g))^{r_s} \right\rangle_g \right\rangle_G^n$$
(B11)

with n equal to p-1 and p respectively. Since  $\xi^* < 0$  it is easy to see how only positive terms of the series survive. Collecting all, we eventually find the complete power expansion for  $R_{1RSB}^{K-SAT}$ :

$$\frac{\alpha}{\beta m} \sum_{l \ge 1} \frac{m^l}{l} \sum_{k_1, \dots, k_l}^{1, \infty} (-\xi^*)^{\sum_{s=1}^l k_s} \prod_{s=1}^l \left( \frac{\prod_{r=1}^{k_s-1} (r-m)}{k_s!} \right) \times \Omega^{(l)} \left[ (1 + \mathbf{Q}(k_1, \dots, k_l))^p - p(1 + \mathbf{Q}(k_1, \dots, k_l)) \mathbf{A}(k_1, \dots, k_l)^{p-1} + (p-1) \mathbf{A}(k_1, \dots, k_l)^p \right]$$
(B12)

where we have defined

$$\mathbf{A}(k_1, ..., k_l) \equiv \left\langle \prod_{s=1}^l \left\langle (1 + J \tanh(\beta g))^{k_l} \right\rangle_g \right\rangle_G$$
(B13)

Again, every term of the expansion is positive for even p and for p odd under condition  $1 + \mathbf{Q}(k_1, ..., k_l) \geq 0$ .

#### APPENDIX C: APPENDIX C

Let us briefly sketch the proof of the existence of the thermodynamic limit of free-energy of the p spin model for p. Let us define a model which interpolates between two non interacting systems with  $N_1$  and  $N_2$  spins respectively, and a system of  $N=N_1+N_2$  spins. Each clause  $\mu=1,...,M$  will belong to the total system with probability t, to the first subsystem with probability  $N_1/N(1-t)$  and to the second subsystem with probability  $N_2/N(1-t)$ . We chose the indices  $i_1^{\mu},...,i_p^{\mu}$  in the following way: for each clause the indices will be i.i.d. with probability t, the indices will be chosen uniformly in the set  $\{1,...,N\}$ , with probability  $(1-t)N_1/N$  the indices will be chosen in  $\{1,...,N_1\}$  and with probability  $(1-t)N_2/N$  in the set  $\{N_1+1,...,N\}$ . Let us consider the free-energy  $F_N(t)=\frac{-1}{N\beta}\log Z(t)$ . A direct calculation of its t-derivative

$$\frac{dF_N(t)}{dt} = -\frac{1}{\beta} \left[ \frac{1}{N^p} \sum_{i_1,\dots,i_p}^{1,N} + \frac{N_1}{N} \frac{1}{N_1^p} \sum_{i_1,\dots,i_p}^{1,N_1} + \frac{N_2}{N} \frac{1}{N_2^p} \sum_{i_1,\dots,i_p}^{N_1+1,N} \right] E\langle \log(1 + \tanh(\beta J)\omega(S_{i_1}...S_{i_p})) \rangle_J. \tag{C1}$$

Expanding the logarithm in series, observing that thanks to the symmetry of the J distribution the odd term vanish, introducing the replica measure and using the convexity of the function  $x^p$  for even p one proves that  $\frac{dF_N(t)}{dt} \leq 0$  which implies sub-additivity  $F_N \leq \frac{N_1}{N}F_{N_1} + \frac{N_2}{N}F_{N_2}$ ; this is in turn is a sufficient condition to the existence of the free-energy density. The same prove applies to the even p random K-SAT model. For odd p we face a difficulty similar to the one in the replica bounds. We can not prove sub-additivity due to the need to consider negative values of the overlaps, and non convexity of  $x^p$  for negative x.

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